arXiv:cond-mat/0003323v1 20 Mar 2000

Dynamic Scaling for First-order Phase Transtions†

Banu Ebru Özoğuz, Yiğit Gündüç and Meral Aydın

Hacettepe University, Physics Department,

06532 Beytepe, Ankara, Turkey

Abstract

The critical behaviour in short time dynamics for the $q = 6$ and 7 state Potts models in two-dimensions is investigated. It is shown that dynamic finite-size scaling exists for first-order phase transitions.

Keywords: First-order phase transition,dynamic scaling, Potts model, finite size scaling, Monte Carlo simulation

†This project is partially supported by Turkish Scientific and Technical Research Council (TÜBİTAK) under the project TBAG-1669.

1 Introduction

It has been shown that [1] for a dynamical relaxation process in which a system, evolving according to a dynamics of model A [2], and is quenched from very high temperature to the critical temperature, there emerges a universal dynamical scaling behaviour already within the short-time regime. This rather unexpected scaling seems to exist, since spatial correlations and correlation time diverge simultaneously as the system approaches long- time regime at the critical temperature. For the short-time regime, the finite-size scaling form of the time evolution of a k-th moment of the magnetization is written as [1]

$$M^{(k)}(t, \epsilon, m_0) \; = \; b^{-k\beta/\nu} \; M^{(k)}(t/\tau(L), b^{1/\nu}\epsilon, b^{x_0} m_0). \tag{1}$$

Here b is the scale change, L is the linear dimension of the system, β, ν are the well known static critical exponents, τ is the autocorrelation time, and $\epsilon = (T - T_c)/T_c$ is the reduced temperature. Short-time dynamic behaviour also requires a new independent critical exponent x_0 which is the scaling dimension of the initial magnetization m_0. It has been shown numerically that dynamic scaling exists [3] even at the very early stages of the relaxation process.

Rigorous formulation of the finite-size scaling for first-order phase transitions [4, 5] resulted in better understanding of the dynamics of the first-order phase transi-

tions. In this formalism it has been shown that the phase transition is governed by the surface tension between the ordered and disordered phases. The system tunnels between these two metastable states and these transitions are observed during simulation studies of the long-term behaviour of the system. For finite systems, undergoing first-order transitions, the autocorrelation time τ for the relaxation process has been calculated [6, 7] for cluster algorithms [8, 9] and is given as

$$\tau \;=\; L^{d/2} \exp(\sigma_{od}\, L^{d-1}), \tag{2}$$

where d is the dimensionality of the system.This form of τ can be used to identify the order of the phase transition.

In a series of previous work [10, 11], behavioral differences between first- and second-order phase transitions have been studied. In these works, empirically distinct change in the time evolution of the operator in initial stages of the simulation gave a clear indication that first- and second-order phase transitions are grouped into two different evolutionary processes. Since short-time dynamic behaviour of second-order phase transitions are well understood in terms of dynamic scaling formalism [1], in analogy with second-order transition, scaling for first-order transitions may be put into more rigorous footing. The success of the finite size scaling arguments and explicit form of τ given in Eq.(2) led us to study the existence of short-time dynamic scaling in first-order phase transitions. In first-order phase transitions the singular-

ities are governed by the volume of the system. Hence in first-order transitions the thermal and magnetic critical indices are replaced by the dimension of the system. Combining this information with Eq.(2), we have formulated dynamic scaling form of various operators in anology with Eq. (1). In this work, our aim is to show that a system exhibiting first-order phase transition obeys well defined dynamic finite-size scaling rules during quenching from disordered state to the infinite lattice transition temperature. We have studied the short-time relaxation processes by using $q = 6$ and 7 state Potts models, which are known to exhibit first-order phase transition. In this model we studied the time evolutions of the order parameter, the largest cluster and the Binder cumulant [12].

2 Model and Method

The Hamiltonian of the q-state Potts model [13, 14] is given as

$$-\beta H = \sum_{<ij>} K\delta_{s_i,s_j} \tag{3}$$

where the spin s can take values $1, \ldots, q$, $\beta = 1/k_BT$ is the inverse temperature, $K = J/(k_BT)$, δ is the Kroneker delta function, and sum is over all nearest-neighbour pairs on two-dimensional lattice. In equilibrium the q-state Potts model is exactly solvable. The critical point locates at $K_c = \log(1 + \sqrt{q})$. In principle, any type

of dynamics can be given to the system to study non-equilibrium time evolution process. In this work, we used nonconserved dynamics of Model A [2]. In order to study dynamic scaling in systems exhibiting first-order phase transitions the following operators are considered:

1. Moments of the order parameter (M)

$$M^{(k)} \;=\; \langle (\frac{q\,\rho^{\alpha}-1}{q-1})^{k} \rangle \tag{4}$$

   $\rho^{\alpha} = N^{\alpha}/L^{d}$, N^{α} being the number of spins with $s = \alpha$, L the linear size and d is the dimensionality of the system.

2. Binder cumulant (B)

$$B \;=\; 1 - \frac{M^{(4)}}{3\,{M^{(2)}}^{2}} \tag{5}$$

3. Largest cluster (C_m)

$$C_m \;=\; \frac{1}{L^{d}} \langle N_{C_m} \rangle \tag{6}$$

N_{C_m} is the number of spins belonging to the largest cluster in each configuration. Largest cluster gives the time evolution of the average of the largest cluster found in each configuration. This quantity scales like the susceptibility. Hence in a first-order phase transition, it grows like volume.

For the first-order phase transitions, since the static critical exponents are replaced by the dimension of the system, rather than calculating the static critical indices, one can test the validity of the dynamic scaling assumption at the initial stages of the simulation and obtain the surface tension as the result of the scaling. For the computational simplicity, the initial magnetization m_0 is set to zero. For second-order phase transitions, the finite-size behaviour of the magnetization is given by Eq.(1). Here, $\beta/\nu = Y_H - d$. Since Y_H and Y_T are equal to the dimension of the system, for first-order phase transitions, the order parameter ($M^{(1)}$), Binder cumulant (B) and the largest cluster (C_m) scale according to

$$f_{L_1}(t/\tau(L_1), 0, L_1) = f_{L_2}(t/\tau(L_2), 0, L_2) \tag{7}$$

where $\tau(L)$ is autocorrelation time of the lattice with the linear size L. Application of this form to data can show scaling for various size lattices. In the following section we have presented our results.

3 Results and Discussions

Following the considerations started in previous section, we have studied the two-dimensional $q = 6$ and 7 state Potts models evolving in time according to dynamics of model A [2]. Our main objective is to observe the dynamic scaling, hence we have

prepared lattices with vanishing order parameter, avoiding the complications due to having an extra parameter x_0. This is achived for $q = 6$ and 7 state Potts models by choosing the lattice sizes as the integer multiples of q. Totally random initial configurations are quenched at the corresponding infinite lattice transition temperature. Simulations are performed on 6 different lattice sizes by using Wolff cluster update algorithm. For each q and L the averages are taken over 10000 different samples. Errors are calculated by dividing the samples into ten subsamples. As the lattice size grows, number of iterations for thermalization grows according to growing tunneling time (Eq. 2). For $q = 7$ and larger lattices up to 30000 iterations are necessary for thermalization. The chosen lattice sizes are $L = 42, 60, 72, 90, 96, 102$ and $L = 35, 49, 63, 77, 91, 105$ for $q = 6$ and $q = 7$ respectively.

The two-dimensional q-state Potts model is known to undergo first-order phase transition for $q > 4$ [15]. Even though the $q = 7$ state Potts model exhibits strong first-order behaviour, the correlation length is about 50 lattice sites. Hence for $q = 7$ [16], the largest lattices are expected to show good scaling behaviour without any need to correction to scaling terms. For smaller lattices, however, one needs to consider the correction to scaling according to the finite-size scaling theory for first-order phase transitions. The general form of the corrections to the scaling can be given as polynomial in $\frac{1}{L^d}$, which can be written as

$$\langle A \rangle_L \;=\; A_0 \,(1 \;+\; \frac{A_1}{L^d} \;+\; \frac{A_2}{L^{2d}} \;+\; \ldots). \tag{8}$$

This form indicates that all of the observables scale if one calculates A_0 by fitting the correction to scaling terms [4, 5, 17]. The correction to scaling plays even more profound role for $q = 6$ state Potts model where the correlation length is larger than even the largest lattice. The correction to scaling for each observable is obtained by fitting the averages, taken over 10000 iterations after the thermalization, to Eq. (8) and the expansion coefficients A_1, A_2,.. are calculated for $q = 6$ and 7.

In Figure 1.a, the time evolution of the order parameter is plotted for $q = 6$. As one can observe, for each lattice size, starting from totally random configuration $m_0 \;=\; 0$, the order parameter evolves to a plato. For large enough lattices, since $Y_H - d$ vanishes for first-order phase transitions, one can expect the same long-term behaviour for all different lattice sizes. In fact this is the case, within the errorbars, for our largest two lattices. In order to see scaling for smaller lattice sizes we have performed long runs, after thermalization, and the correction to scaling terms (Eq. 8) are fitted to the order parameter values. In figures 1.a and 1.b the raw data and the scale form is presented for $q = 6$ and 7 respectively. Figures 1.c and 1.d show the scaled forms of the data in figures 1.a and 1.b respectively. For $q = 7$, the correction to scaling is almost negligible for lattices larger than $L = 65$.

	q = 6			q = 7		
M	0.0084	±	0.0011	0.0185	±	0.0015
B	0.0076	±	0.0004	0.015	±	0.002
C_m	0.0084	±	0.0011	0.0175	±	0.0015

Table 1: $2\,\sigma_{od}$ for $q = 6$ and 7

Similarly, for the averages of the maximum cluster, which is expected to grow like the volume, we have observed that similar scaling behaviour exists. Figures 2.a and 2.b are plots of the Monte Carlo data for $q = 6$ and $q = 7$ respectively. Figures 2.c and 2.d are the scaled form of the above mentioned data.

The last quantity that we have observed is the Binder cumulant. Binder cumulant is a scaling function and also is a ratio of two quantities of equal anomolous dimensionality. Hence, correction to scaling terms are almost negligible even for very small lattices.

These scaling studies enable us to calculate the order-disorder surface tension $2\sigma_{od}$. The surface tensions $2\sigma_{od}$ of $q = 6$ and $q = 7$ state Potts models are calculated from the autocorrelation time of the relaxation processes for the observables. In Table 1. we have presented $2\,\sigma_{od}$ which are obtained from the relaxation of three different quantities. Depending on the quantity, the value of the surface tension is observed to vary slightly. Nevertheless, the surface tension, within errorbars, is 0.008 ± 0.001 and 0.017 ± 0.004 for $q = 6$ and $q = 7$ respectively. The error on the surface tension

can be taken as the fluctuation of the values obtained using different operators.

4 Conclusions

In conclusion we have numerically simulated the dynamic relaxation process of the two-dimensional $q = 6$ and 7 state Potts models starting from random initial states with vanishing initial order parameter. Here in this preliminary work we have investigated the dynamical scaling properties of the first-order phase transitions. This work is based on two well established facts that the autocorrelation time of the critical relaxations in first-order phase transitions are given by the instanton calculations [7] and all infinities of the thermodynamic quantities are governed by the volume of the system [4, 5, 17]. Under these assumptions one may expect that any thermodynamical quantity exhibits dynamical scaling considering the correction to scaling terms.

We have demonstrated that for first-order phase transitions a universal scaling behaviour emerges already in the macroscopic short-time regime of the dynamical evolution. This scaling behaviour resembles closely dynamic scaling which seems to exist in second-order phase transitions. Furthermore, such a scaling opens new and alternative methods of calculating surface tension and it can be used to distinguish weak-first-order phase transitions from the second-order one.

References

[1] H.K.Janssen, B. Schoub and B. Schmittmann Z. Phys. B73 (1989) 539.

[2] P.C.Hohenberg and B. I. Halperin Rev. Mod. Phys. B49 (1977) 435.

[3] B. Zheng, Int. J. Mod. Phys. B 12 (1998) 1419.

[4] C. Borgs and R. Kotecky, J. Stat. Phys. 61 (1990) 79.

[5] C. Borgs, R. Kotecky and S. Miracle-Sole, J. Stat. Phys. 62 (1991) 529.

[6] K. Binder, Phys. Rev. B 25 (1982) 1699.

[7] J. C. Niel, J. Zinn-Justin, Nucl. Phys. B280 (1987) 355.

[8] R. H. Swendsen and J. S. Wang, Phys. Rev. Lett. 58 (1987) 86.

[9] U. Wolff, Phys. Rev. Lett. 62 (1989) 361.

[10] M. Aydın and Y. Gündüç Physica A 232 (1996) 265.

[11] F. Yasar, Y. Gündüç, M. Aydın and T. Çelik Physica A 255 (1998) 430.

[12] K. Binder, Phys. Rev. Lett. 47 (1981) 693.

[13] R. B. Potts, Proc. Camb. Phil. Soc. 48 (1952) 106.

[14] F. Y. Wu, Rev. Mod. Phys. 54 (1982) 235.

[15] R. J. Baxter, J. Phys. C6 (1973) L445.

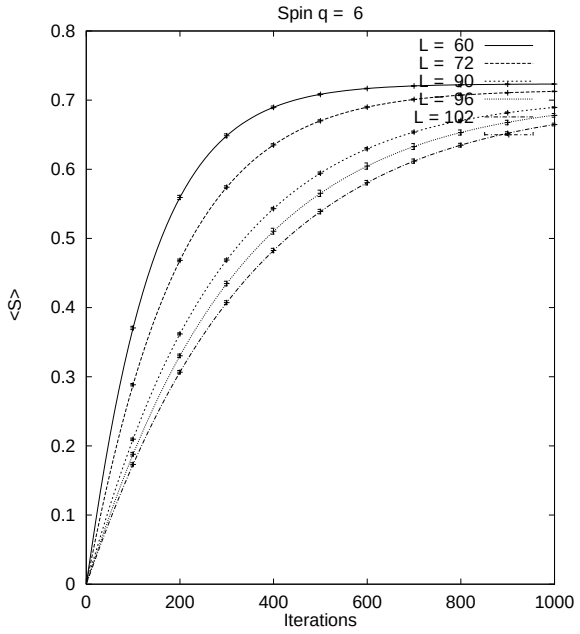
[16] E. Buffenoir and S. Wallon, J. Phys. A26 (1993) 3045.

[17] A. Billoire, Nucl. Phys. (Proc. Suppl.) B42 (1995) 21.

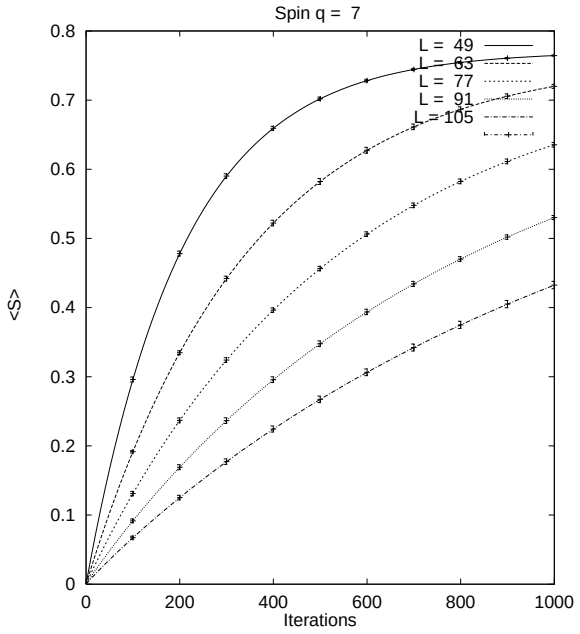
Figure captions

Figure 1. (a) and (b) are the time evolution of the order parameter M, and (c) and (d) are their scaled form for $q = 6$ and 7-state Potts model respectively. (The errorbars are omitted from the scaled forms for clarity of the figures.)

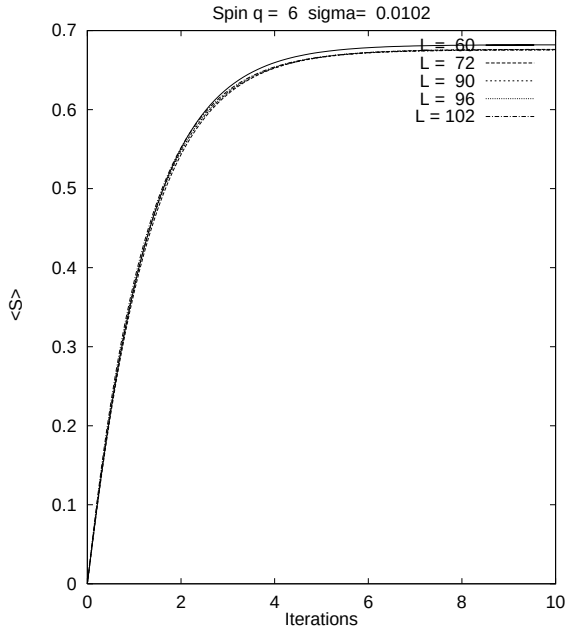
Figure 2. Same as fig. 1 but plots are for the maximum clusters.



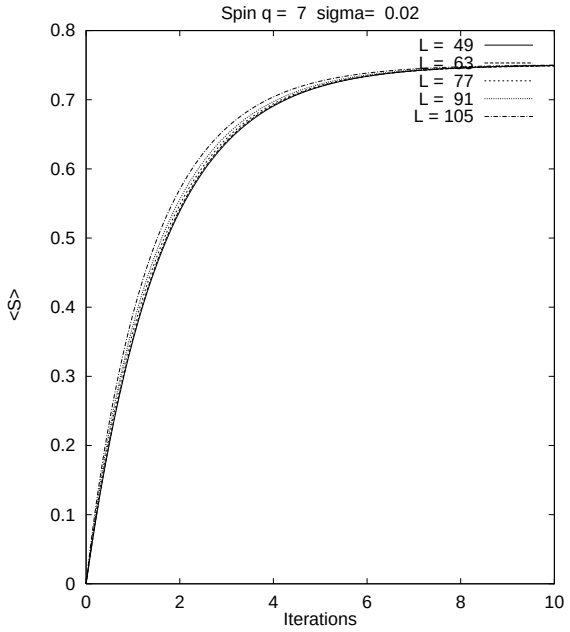
(a)



(b)

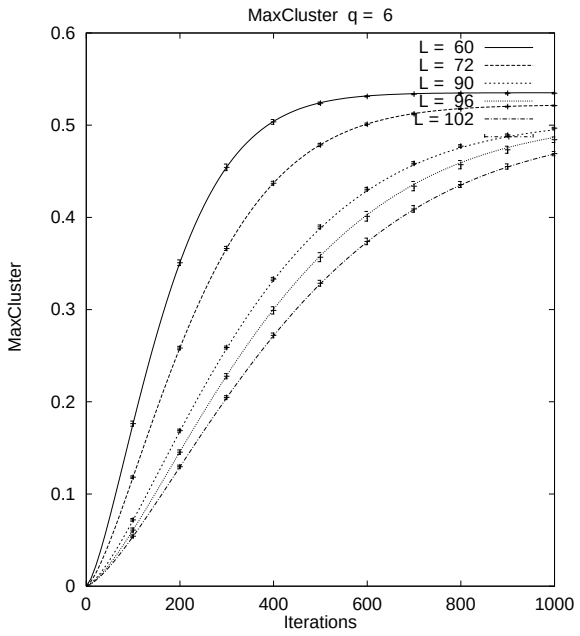


(c)

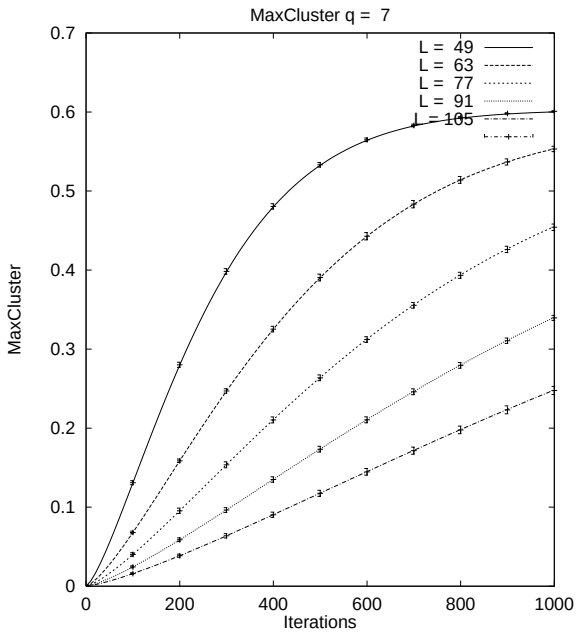


(d)

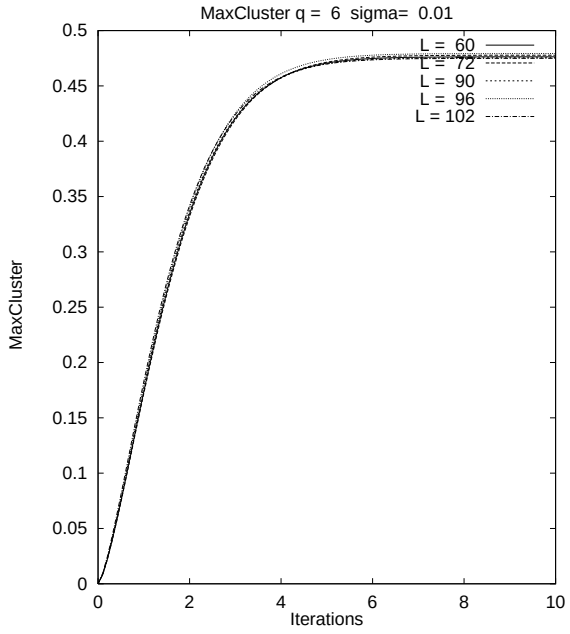
Figure 1:



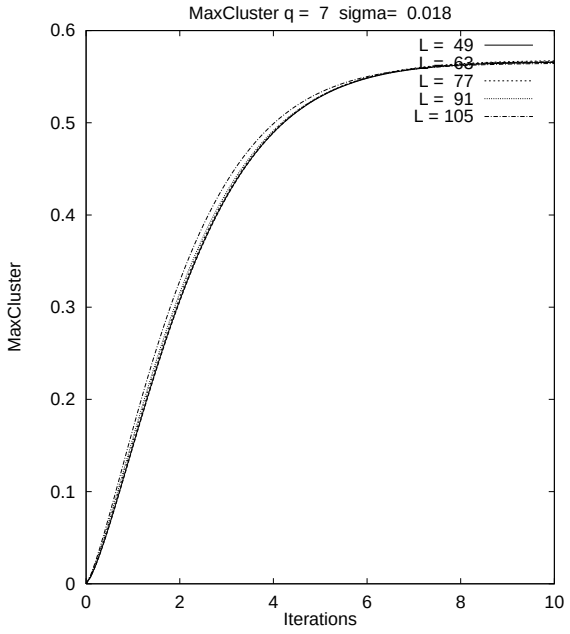
(a)



(b)

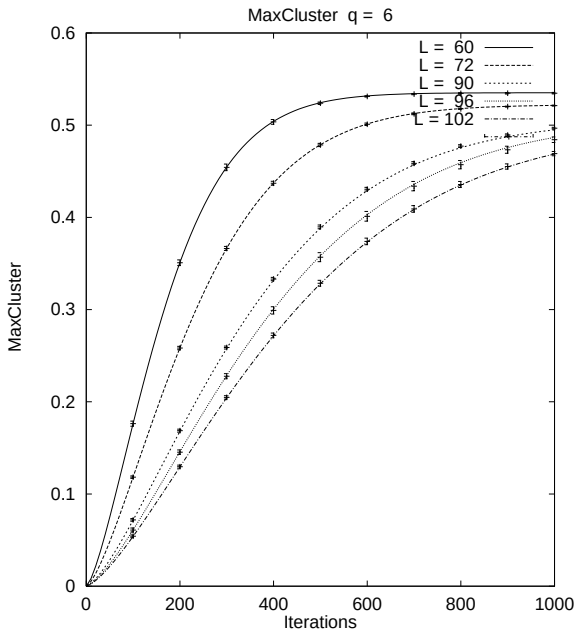


(c)

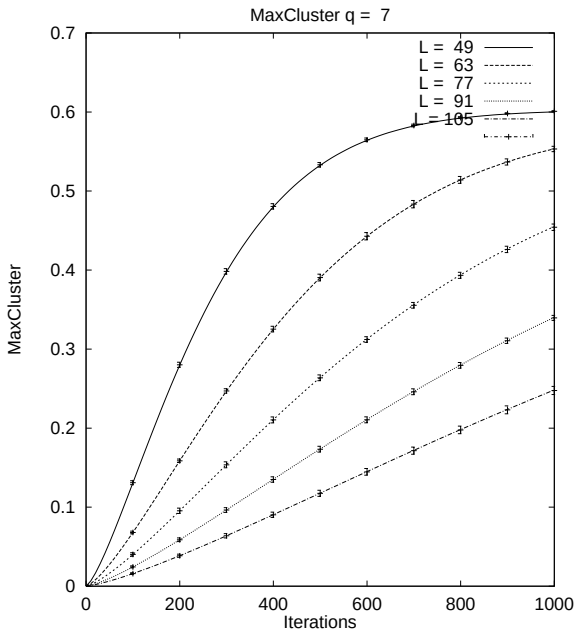


(d)

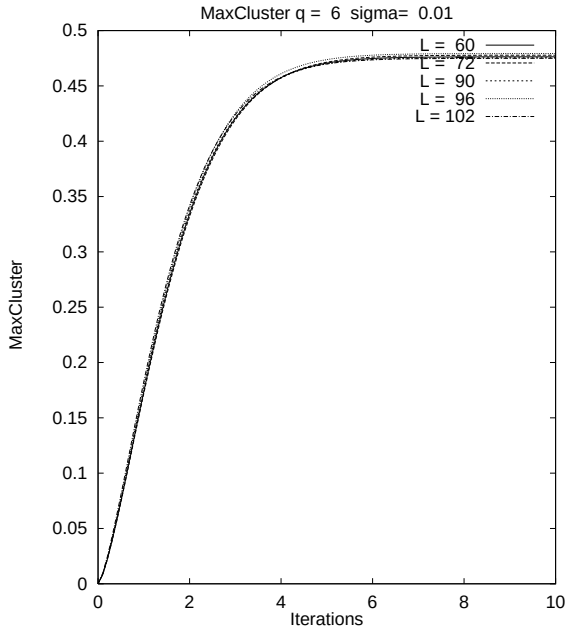
Figure 2:



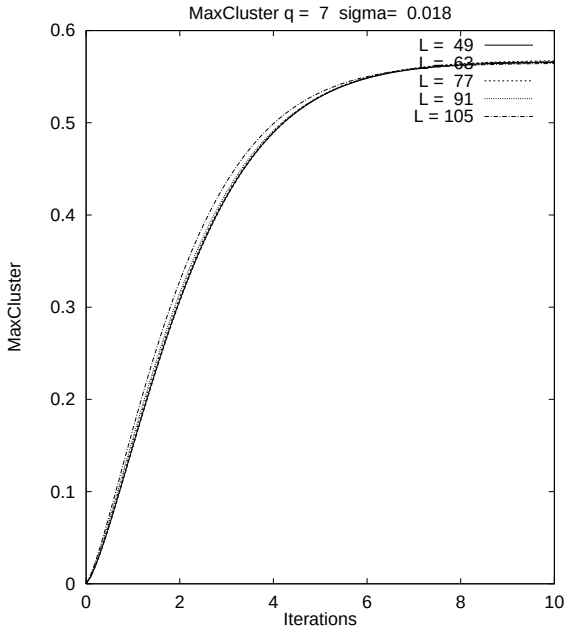
(a)



(b)



(c)



(d)

Figure 2: